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DFT/TD-DFT Investigation of Optical Absorption Spectra, Electron Affinities, and Ionization Potentials of Mono-Nitrated Benzanthrones [Abstract]

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Density functional theory (DFT) method B3LYP with basis sets 6-311+G(d,p), 6-31G(d) and 6-311G(d,p) have been used to compute molecular structures, UV–vis absorption spectra, electron affinities (EAs), and ionization potentials (IPs) of benzanthrone and 1-, 2-, 3-, 9-, 10-, and 11-nitrobenzanthrones. With the use of the time-dependent TD-B3LYP/6-311G(d,p) approach, the UV/vis absorption spectral bands, vertical excitation energies and oscillator strengths was studied. The calculated vertical excitation energies lie within <0.15 eV of the observed values. In comparison to benzanthrone, calculated absorption spectra of nitrated nitrobenzanthrones show red-shifting to >383 nm, which is correlated to their relative reactivity. Detailed clarification of the singlet-singlet excited states (and energies) are made. The calculated electron affinities are ∼0.5 eV greater than in benzanthrone (BA); being in the order 3-NBA > 10-NBA > 1-NBA > 2-NBA > 9-NBA > 11-NBA > BA. Similarly, ionization potentials follow a very close order in nitro-BAs. The calculated EAs and IPs implicate both reductive and oxidative pathways on transformation to mutagenic metabolites. The implications of the results are discussed in the context of their differential mutagenic potencies.